

Some analytic results on the FPU paradox

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Abstract

We present some analytic results aiming at explaining the lack of thermalization observed by Fermi Pasta and Ulam in their celebrated numerical experiment. In particular we focus on results which persist as the number N of particles tends to infinity. After recalling the FPU experiment and some classical heuristic ideas that have been used for its explanation, we concentrate on more recent rigorous results which are based on the use of (i) canonical perturbation theory and KdV equation, (ii) Toda lattice, (iii) a new approach based on the construction of functions which are adiabatic invariants with large probability in the Gibbs measure.

1 Introduction

In their celebrated numerical experiment Fermi Pasta and Ulam [FPU65], being interested in the problem of foundation of statistical mechanics, studied the dynamics of a chain of nonlinear oscillators. In particular they studied the evolution of the energies of the normal modes and their time averages. FPU considered initial data with all the energy in the first Fourier mode and observed that (1) the harmonic energies seem to have a recurrent behaviour (2) the time averages of the harmonic energies quickly relaxes to a distribution which is exponentially decreasing with the wave number (FPU packet of modes). This was quite surprising since, from the principles of statistical mechanics, the solution was expected to explore the whole phase space and the energies of the normal modes were expected to relax to equipartition.

Subsequent numerical and analytic investigations tackled the problem of understanding such a behaviour and of understanding whether or not it persists as the number N of the particles tends to infinity. In particular the interesting regime is that of the thermodynamic limit in which the specific energy is kept fixed while $N \rightarrow \infty$. Indeed, in order to be relevant for the foundation of statistical mechanics the FPU paradox (namely the phenomena described above) has to persist in such a limit.

The aim of the present paper is to present a short review of the status of the research, focusing only on analytic results and in particular to a couple of results recently obtained by the authors [BM14, MBC14].

The paper is organized as follows: in sect. 2 we recall the FPU numerical results (we add only one further very old numerical result showing the existence of a threshold for thermalization). In sect. 2.5 we will discuss some theoretical ideas which have been used in order to try to explain and to understand the FPU paradox. In particular we will discuss (1) the relation between FPU lattice and KdV equation, (2) the use of KAM theory and canonical perturbation theory (and Nekhoroshev's theorem) in the context of FPU dynamics. In Sect. 2.6 we present some rigorous results that have been obtained in the last ten years on the problem. In Sect.5.1 we present a recent result which exploits the vicinity of the Toda lattice and the FPU chain in order to improve known results of the lifetime of the FPU packet. Finally, in Sect.6 we will present an averaging theorem for the FPU chain valid in the thermodynamic limit. This last result in particular deals with a slightly different problem, namely the exchange of energy among the different degrees of freedom when one starts with an initial datum belonging to a set of large Gibbs measure. We conclude the paper with a short discussion Sect. 7.

2 Introduction to FPU paradox

The Hamiltonian of the FPU-chain can be written, in suitably rescaled variables, as

$$H_{FPU} = H_0 + H_1 + H_2 \quad (2.1)$$

where

$$\begin{aligned} H_0 &\stackrel{\text{def}}{=} \sum_j \left(\frac{p_j^2}{2} + \frac{(q_{j+1} - q_j)^2}{2} \right), \\ H_1 &\stackrel{\text{def}}{=} \frac{1}{3!} \sum_j (q_{j+1} - q_j)^3 \\ H_2 &\stackrel{\text{def}}{=} \frac{A}{4!} \sum_j (q_{j+1} - q_j)^4, \end{aligned}$$

where (p, q) are canonically conjugated variables. We will consider the case of periodic boundary conditions, i.e. $q_{-N-1} = q_{N+1}$ and $p_{-N-1} = p_{N+1}$.

In order to introduce the Fourier basis consider the vectors

$$\hat{e}_k(j) = \hat{e}_k(j) = \begin{cases} \frac{1}{\sqrt{N+1}} \sin\left(\frac{jk\pi}{N+1}\right), & k = 1, \dots, N, \\ \frac{1}{\sqrt{N+1}} \cos\left(\frac{jk\pi}{N+1}\right), & k = -1, \dots, -N, \\ \frac{1}{\sqrt{2N+2}}, & k = 0, \\ \frac{(-1)^j}{\sqrt{2N+2}}, & k = -N-1. \end{cases} \quad (2.2)$$

Unless specifically needed, we will not specify the set where the indexes j , and k vary.

Introducing the Fourier variables (\hat{p}_k, \hat{q}_k) by

$$p_j = \sum_k \hat{p}_k \hat{e}_k(j) , \quad q_j = \sum_k \hat{q}_k \hat{e}_k(j) \quad (2.3)$$

with

$$\omega_k = 2 \sin \left(\frac{|k|\pi}{2(N+1)} \right) . \quad (2.4)$$

the system takes the form

$$H = H_0 + H_1 + H_2 \quad (2.5)$$

where

$$H_0(\hat{p}, \hat{q}) = \sum_k \frac{\hat{p}_k^2 + \omega_k^2 \hat{q}_k^2}{2} , \quad H_1 = H_1(\hat{q}) , \quad H_2 = H_2(\hat{q}) . \quad (2.6)$$

We also introduce the harmonic energies

$$E_k = \frac{\hat{p}_k^2 + \omega_k^2 \hat{q}_k^2}{2} ,$$

and their time averages

$$\langle E_k \rangle(T) := \frac{1}{T} \int_0^T E_k(t) dt . \quad (2.7)$$

We will often use also the *specific harmonic energies* defined by

$$\mathcal{E}_k := \frac{E_k}{N} . \quad (2.8)$$

We recall that according to the principles of classical statistical mechanics, at equilibrium, each of the harmonic oscillators should have an energy equal to β^{-1} , $\beta = (k_b T)^{-1}$ being the standard parameter entering in the Gibbs measure (and k_b being the Boltzmann constant). Furthermore, if the system has good statistical properties, the time averages of the different quantities should quickly relax to their equilibrium value.

Fermi Pasta and Ulam studied the time evolution¹ of E_k and of $\langle E_k \rangle$. Figure 1 shows the results of the numerical computations by FPU; the initial data are chosen with $E_1(0) \neq 0$ and $E_k(0) = 0$ for any $|k| > 1$.

From Figure 1 one sees that the energy flows quickly to some modes of low frequency, but after a short period it returns almost completely to the first mode, in the right part of the figure the final values of $\langle E_k \rangle(t)$ are plotted in a linear scale. The final distribution turns out to be exponentially decreasing with k .

If one continues the integration one sees that the phenomenon repeats almost identically for a very long time (see figure 2).

¹Actually FPU studied the case of Dirichlet boundary conditions, but as is well known, such a case can be considered as a subcase of that of periodic boundary conditions.

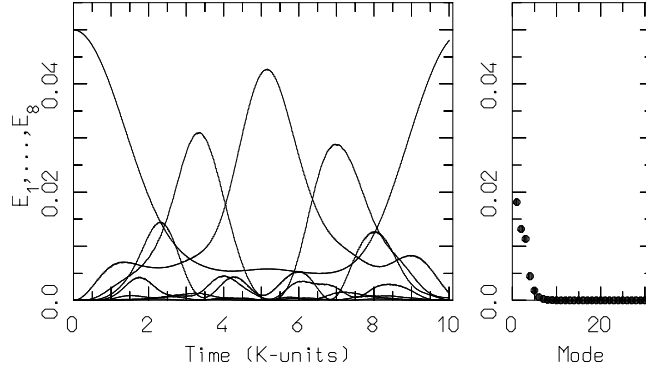


Figure 1: Energy per mode and final value of their time averages.

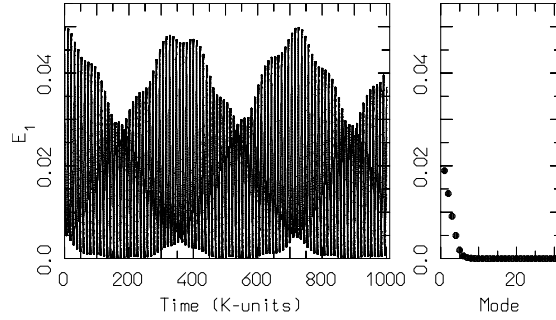


Figure 2: Energy of the first mode and final value of $\langle E_k \rangle(t)$ at longer time scales.

In figure 3 the averages $\langle E_k \rangle(t)$ are plotted versus time in a semi-log scale. Figure 3 corresponds to initial data with small energy, and one sees that the quantities $\langle E_k \rangle(t)$ quickly relax to well defined values, say \bar{E}_k . Such values depend on k , and, as shown by figure 2, decay exponentially.

To describe the situation with the words by Fermi Pasta and Ulam “The result shows very little, if any, tendency towards equipartition of energy among the degrees of freedom.” This is what is usually known as the Fermi Pasta Ulam paradox.

It is interesting to investigate the behaviour of the system when the energy per particle is increased. This is described in the second of figures 4 from which one sees that the FPU paradox disappears in this regime: here equipartition is quickly reached.

FPU numerical experiment has originated a huge amount of scientific research and in particular subsequent numerical computations have established the shape of the packet of modes to which energy flows (see e.g. [BGG04])

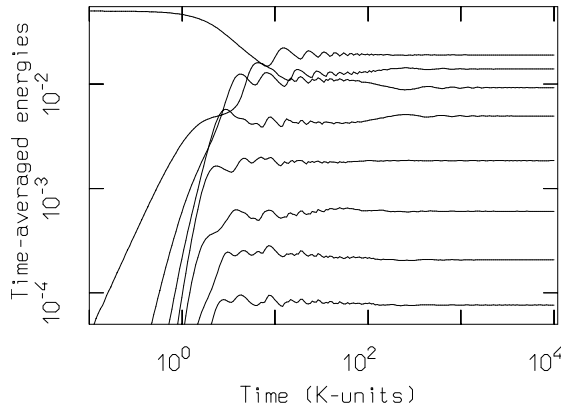


Figure 3: $\langle E_k \rangle(t)$ versus time.

and have put into evidence that the FPU packet is only metastable [FMM⁺82], namely that after a quite long time, whose precise length is not yet precisely established, the system relaxes to equipartition (see e.g. [BGP04, BP11]).

3 Theoretical analysis

We remark that the *theoretical* understanding of the FPU paradox would be absolutely fundamental: indeed it is clear that the phenomenon has some relevance for the foundation of statistical mechanics if it persists in the thermodynamic limit, i.e. in the limit in which the number of particles $N \rightarrow \infty$ while the energy per mode, namely $\sum_k E_k/N$ is kept fixed. Of course numerics can give some indications, but a definitive result can only come from a theoretical result, which is the only one able to reach the limit $N = \infty$.

3.1 KdV

One of the first attempts to explain the FPU paradox has been on the use of the Kortweg de Vries equation (KdV). The point is that on the one hand KdV is known to approximate the FPU and on the other one KdV is also known to be integrable, so that it displays (in suitable variables) a recurrent behaviour.

We now recall briefly the way KdV is introduced as a modulation equation for the FPU. We also restrict to the subspace

$$\sum_j q_j = 0 = \sum_j p_j \quad (3.1)$$

which is invariant under the dynamics. The idea is to consider initial data with long wave and small amplitude, namely to interpolate the difference $q_j - q_{j+1}$

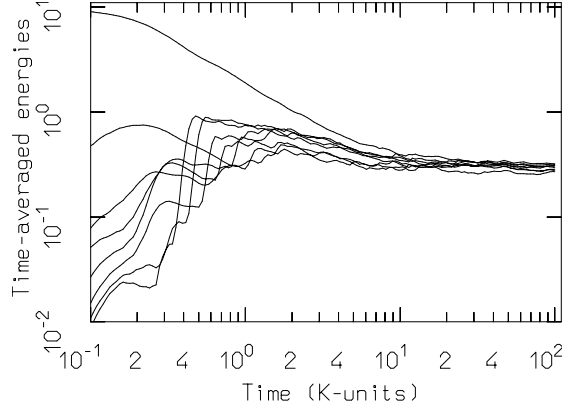


Figure 4: $\langle E_k \rangle(t)$ versus time at large energy.

through a smooth small function slowly changing in space (and time). This is obtained through an Ansatz of the form

$$q_j - q_{j+1} = \epsilon u(\mu j, t), \quad \mu := \frac{1}{N}, \quad \epsilon \ll 1 \quad (3.2)$$

with u periodic of period 2. It turns out that in order to fulfill the FPU equations, the function u should have the form

$$u(x, t) = f(x - t, \mu^3 t) + g(x + t, \mu^3 t)$$

with $f(y, \tau)$ and $g(y, \tau)$ fulfilling the equations

$$f_\tau + \frac{\mu^2}{\epsilon} f_{yyy} + f f_y = O(\mu^2), \quad g_\tau - \frac{\mu^2}{\epsilon} g_{yyy} - g g_y = O(\mu^2), \quad (3.3)$$

namely, up to higher order corrections, a couple of KdV equations with dispersion of order μ^2/ϵ describe the system. Now, it is of the year 1965 the celebrated paper by Zabuski and Kruskal on the dynamics of the KdV equation which was the starting point of soliton theory and led in particular to the understanding that KdV is integrable. Thus, the enthusiasm for the discovery of such a beautiful and important phenomenology, led the idea that also the FPU paradox could be explained by the fact that the dynamics of the FPU is described in some limit by an integrable equation.

In order to transform such a heuristic idea into a theorem one should fill two gaps, the first one consists in showing that in the KdV equation a phenomenon of the kind of the formation and persistence of the packet of modes occurs, and the second one consisting in showing that the solutions of the KdV equation actually describe well the dynamics of the FPU, namely that the higher order corrections neglected in (3.3), are actually small.

Both problems can be solved in the case $\epsilon = \mu^2$, in which the KdV equation turns out to be the standard one. Indeed the action angle coordinates for the

KdV equation with periodic boundary conditions have been constructed and studied in detail [KP03] and with their help one can show that if, in the KdV equation one puts all the energy in the first Fourier mode, then the energy remains forever localized in an exponentially localized packet of Fourier modes.

However, if one wants to take the limit $N \rightarrow \infty$ while keeping ϵ fixed (as needed in order to get a results valid in the thermodynamic limit), one has to study the dispersionless limit of the KdV equation and very little is known on the behaviour of action angle variables in this limit, so that the standard theory becomes inapplicable. Thus we can say that, **in the KdV equation** the phenomenon of formation and persistence of the packet is not explained in the limit corresponding to the thermodynamic limit of the FPU lattice.

The second problem is also far from trivial, since the perturbation terms of (3.3) contain higher order derivatives, so we are dealing with a singular perturbation of KdV and the proof of theorems connecting the solutions of KdV and the solutions of FPU have only recently been obtained [SW00, BP06].

3.2 KAM theory and canonical perturbation theory

Izrailiev and Chirikov [IC66] in 1966 suggested to explain the behaviour observed by FPU through KAM theory. We recall that KAM theory deals with perturbations of integrable systems and ensures that, provided the perturbation is small enough, most of the invariant tori in which the phase space of the unperturbed system is foliated persist in the complete system. In the case of FPU of course the integrable system is the linearized chain and the perturbation is provided by the nonlinearity, so the size of the nonlinearity increases with the energy of the initial datum and KAM theory should apply for energy smaller than some N -dependent threshold ϵ_N . This approach has the remarkable feature of potentially explaining the recurrent behaviour observed by FPU and also the fact that it disappears for large energy.

From the argument of Izrailiev and Chirikov (based on Chirikov's criterion of overlapping of resonances) one can extract also an explicit estimate of the threshold which should go to zero like $N^{-4} \equiv \mu^4$. Such an estimate is derived by Izrailiev and Chirikov by considering initial data on high frequency Fourier mode, while they do not deduce any explicit estimate for the case of initial data on low frequency modes. Their argument has been extended to initial data on low frequency Fourier modes by Shepeliansky [She97] leading to the claim that also corresponding to such kind of initial data FPU phenomenon should disappear as $N \rightarrow \infty$, however a subsequent reanalysis of the problem has led to different conclusions [Pon05], so, at least, we can say that the situation is not yet clear.

We emphasize that the actual application of KAM theory to the FPU lattice is quite delicate since the hypotheses of KAM theory involve a Diophantine type nonresonance condition and also a nondegeneracy condition. The two conditions have been verified only much later by Rink [Rin01] (see also [Nis71, HK08a]). Then one has to estimate the dependence of the threshold ϵ_N on N and it turns out that a rough estimate gives that ϵ_N goes to zero exponentially with

N (essentially due to the Diophantine type nonresonance condition).

In order to weaken this condition on ϵ_N , Benettin, Galgani, Giorgilli and collaborators [BGG85b, BGG85a, BGG87, BGG89, GGMV92, BG93] started to investigate the possibility of using averaging theory and Nekhoroshev's theorem to explain the FPU paradox. This a quite remarkable change of point of view, since averaging theory and Nekhoroshev's theorem give results controlling the dynamics over long, but finite times, so such a point of view leaves open the possibility that the FPU paradox disappears after a long but finite time, which is what is actually seen in numerical investigations (see also the remarkable theoretical paper [FMM⁺82]). Results along this line have been obtained for chains of rotators ([BGG85b, BG93]) and FPU chains with alternate masses [GGMV92, BG93]. An application to the true FPU model is given in the next section.

4 Some rigorous results

4.1 KdV and FPU

The unification of the two points of view above has been obtained in the paper [BP06], in which canonical perturbation theory has been used in order to deduce a couple of KdV equation playing the role of resonant normal form for the FPU lattice and this has been used in order to describe the phenomenon of formation and metastability of the FPU packet. We briefly recall the result of [BP06].

We consider here the case of periodic boundary conditions. Consider a state of the form (3.2) and write the equation for the evolution of the function u , then it turns out that such an equation is a Hamiltonian perturbation of the wave equation, so one can use canonical perturbation theory for PDEs in order to simplify the equation. Passing to the variables f, g the normal form turns out to be the Hamiltonian of a couple of non interacting KdV equations. In [BP06] a rigorous theory estimating the error was developed, and the main results of that paper are contained in Theorem 4.1 and Corollary 4.2 below.

Consider the KdV equation

$$f_\tau + f_{yyy} + f f_y = 0 ,$$

it is well known [KP03] that if the initial datum extends to a function analytic in a complex strip of width σ , then the solution (as a function of the space variable y) is also analytic (in general in a smaller complex strip).

Consider now a couple of solutions f, g of KdV with analytic initial data and let $q_j^{KdV}(t)$ be the unique sequence such that

$$\begin{aligned} q_j^{KdV}(t) - q_{j+1}^{KdV}(t) &= \mu^2 [f(\mu(j-t), \mu^3 t) + g(-\mu(j+t), \mu^3 t)] , \\ \sum_j q_j^{KdV}(t) &\equiv 0 , \end{aligned} \quad (4.1)$$

where, as above, $\mu := N^{-1}$. Then the result is that q_j^{KdV} approximates well the true solution of the FPU lattice.

Let $q_j(t)$ be the solution of the FPU equations with the initial data $q_j(0) = q_j^{KdV}(0)$, $\dot{q}_j(0) = \dot{q}_j^{KdV}(0)$; denote by $E_k(t)$ the energy in the k^{th} Fourier mode of the solution of the FPU with such initial datum and $\mathcal{E}_k := E_k/N$.

The following theorem holds

Theorem 4.1. *[BP06] Fix an arbitrary $T_f > 0$. Then there exists μ_* such that, if $\mu < \mu_*$ then for all times t fulfilling*

$$|t| \leq \frac{T_f}{\mu^3} \quad (4.2)$$

one has

$$\sup_j |r_j(t) - r_j^{KdV}(t)| \leq C\mu^3, \quad (4.3)$$

where $r_j := q_j - q_{j+1}$ and similarly for r_j^{KdV} . Furthermore, there exists $\sigma > 0$ s.t., for the same times, one has

$$\mathcal{E}_k(t) \leq C\mu^4 e^{-\sigma|k|} + C\mu^5. \quad (4.4)$$

Exploiting known results on the dynamics of KdV (and Hill's operators [Pös11]) one gets the following corollary which is directly relevant to the FPU paradox.

Corollary 4.2. *Fix a positive R and a positive T_f , then there exists a positive constant μ_* , with the following property: assume $\mu < \mu_*$ and consider the FPU system with an initial datum fulfilling*

$$\mathcal{E}_1(0) = \mathcal{E}_{-1}(0) = R^2\mu^4, \quad \mathcal{E}_k(0) \equiv \mathcal{E}_k(t)|_{t=0} = 0, \quad \forall |k| \neq 1, \quad (4.5)$$

Then, along the corresponding solution, equation (4.4) holds for the times (4.2).

Furthermore there exists a sequence of almost periodic functions $\{F_k\}$ such that, defining the specific energy distribution

$$\mathcal{F}_k = \mu^4 F_k, \quad (4.6)$$

one has

$$|\mathcal{E}_k(t) - \mathcal{F}_k(t)| \leq C_2\mu^5, \quad |t| \leq \frac{T_f}{\mu^3}. \quad (4.7)$$

Remark 4.3. *One can show that the following limit exists*

$$\bar{F}_k := \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T F_k(t) dt. \quad (4.8)$$

It follows that up to a small error the time average of $\mathcal{E}_k(t)$ relaxes to the limit distribution obtained by rescaling \bar{F}_k . Of course \bar{F}_k is exponentially decreasing with k , but one can also show that actually one has $\bar{F}_k \neq 0 \quad \forall k \neq 0$

The strong limitation of the above results rests in the fact that they only apply to initial data with specific energy of order μ^4 , thus they do not apply to the thermodynamic limit.

4.2 Longer time scales with less energy

We present here a result by Hairer and Lubich [HL12] which is valid in a regime of specific energy smaller than that considered above, but controls the dynamics for longer time scales. The proof of the result is based on the technique of modulated Fourier expansion developed by the authors and collaborators. In some sense such a technique can be considered as a variant of classical perturbation theory. The key tool that they use for the proof is an accurate analysis of the small denominators entering in the perturbative construction.

To be precise [HL12] deals with the case of periodic boundary conditions.

Theorem 4.4. *There exist positive constants R_* , N_* , T , with the following property: consider the FPU system with an initial datum fulfilling (4.5) with $R < R_*$. Then, along the corresponding solution, one has*

$$\mathcal{E}_k(t) \leq R^2 \mu^4 R^{2(|k|-1)} , \quad \forall 1 \leq |k| \leq N , \quad \forall |t| \leq \frac{T}{\mu^2 R^5} . \quad (4.9)$$

It is interesting to compare the time scale covered by this theorem with the time scale of Corollary 4.2. It is clear that the time scale (4.9) is longer than (4.2) as far as

$$R < N^{-1/5} \quad (4.10)$$

(where we made the choice $T_f := T$), namely in a regime where the specific energy goes to zero faster than in the Theorem 4.1.

One has also to remark that in Theorem 4.4 one gets an exponential decay of the Fourier modes valid for all k 's (the term of order μ^5 present in (4.4) is here absent).

5 Toda lattice

It is well known that close to the FPU lattice there exists a remarkable integrable system, namely the Toda lattice [Tod67, Hén74] whose Hamiltonian is given by

$$H_{Toda}(p, q) = \frac{1}{2} \sum_j p_j^2 + \sum_j e^{q_j - q_{j+1}} , \quad (5.1)$$

(we consider the case of periodic boundary conditions), so that one has

$$H_{FPU}(p, q) = H_{Toda}(p, q) + (A - 1)H_2(q) + H^{(3)}(q),$$

where

$$H_l(q) := \sum_j \frac{(q_j - q_{j+1})^{l+2}}{(l+2)!} , \quad \forall l \geq 2 ,$$

$$H^{(3)} := - \sum_{l \geq 3} H_l ,$$

which shows the vicinity of H_{FPU} and H_{Toda} .

The idea of exploiting the Toda lattice in order to deduce information on the dynamics of the FPU chain is an old one; however in order to make it effective, one has first to deduce information on the dynamics of the Toda lattice itself, and this is far from trivial. The most obvious way to proceed consists in constructing action angle coordinates for the Toda lattice and using them to study the dynamics. An important result in this program was obtained by Henrici and Kappeler [HK08b, HK08a] who constructed action angle coordinates and Birkhoff coordinates (a kind of cartesian action angle coordinates) showing that, for any N , such coordinates are globally analytic (see Theorem 5.1 below for a precise statement). However the construction by Henrici and Kappeler is not uniform in the number of particles N , thus it is not possible to exploit it directly in order to get results for the FPU paradox in the limit $N \rightarrow \infty$.

Results on the behaviour of the integrable structure of Toda for large N have been recently obtained in a series of papers [BGPU03, BKP09, BKP13b, BKP13a, BM14]. In particular in [BKP09, BKP13b, BKP13a], exploiting ideas from [BGPU03], it has been shown that as $N \rightarrow \infty$ the actions and the frequencies of the Toda lattice are well described by the actions and the frequencies of a couple of KdV equations, at least in a regime equal to that of Theorem 4.1, namely of specific energy of order μ^4 .

Further results (exploiting some ideas from [BKP13b, BKP13a, BKP09]) directly applicable to the FPU metastability problem have been obtained in [BM14] and now we are going to present them. In [BM14] the regularity properties of the Birkhoff map, namely the map introducing Birkhoff coordinates for the FPU lattice, have been studied and lower and upper bounds to the radius of the ball over which such a map is analytic have been given.

To come to a precise statement we start by recalling the result by Henrici and Kappeler.

Consider the Toda lattice in the submanifold (3.1) and introduce the linear Birkhoff variables

$$X_k = \frac{\hat{p}_k}{\sqrt{\omega_k}}, \quad Y_k = \sqrt{\omega_k} \hat{q}_k, \quad |k| = 1, \dots, N \quad (5.2)$$

using such coordinates, H_0 takes the form

$$H_0 = \sum_{|k|=1}^N \omega_k \frac{X_k^2 + Y_k^2}{2}. \quad (5.3)$$

With an abuse of notations, we re-denote by H_{Toda} the Hamiltonian (5.1) written in the coordinates (X, Y) .

Theorem 5.1 ([HK08c]). *For any integer $N \geq 2$ there exists a global real analytic canonical diffeomorphism $\Phi_N : \mathbb{R}^{2N} \times \mathbb{R}^{2N} \rightarrow \mathbb{R}^{2N} \times \mathbb{R}^{2N}$, $(X, Y) = \Phi_N(x, y)$ with the following properties:*

- (i) The Hamiltonian $H_{Toda} \circ \Phi_N$ is a function of the actions $I_k := \frac{x_k^2 + y_k^2}{2}$ only, i.e. (x_k, y_k) are Birkhoff variables for the Toda Lattice.
- (ii) The differential at the origin is the identity: $d\Phi_N(0,0) = \mathbb{1}$.

In order to state the analyticity properties fulfilled by the map Φ_N as $N \rightarrow \infty$ we need to introduce suitable norms: for any $\sigma \geq 0$ define

$$\|(X, Y)\|_\sigma^2 := \frac{1}{N} \sum_k e^{2\sigma|k|} \omega_k \frac{|X_k|^2 + |Y_k|^2}{2} \quad (5.4)$$

We denote by $B^\sigma(R)$ the ball in $\mathbb{C}^{2N} \times \mathbb{C}^{2N}$ of radius R and center 0 in the topology defined by the norm $\|\cdot\|_\sigma$. We will also denote by $B_\mathbb{R}^\sigma := B^\sigma(R) \cap (\mathbb{R}^{2N} \times \mathbb{R}^{2N})$ the *real* ball of radius R .

Remark 5.2. We are particularly interested in the case $\sigma > 0$ since, in such a case, states with finite norm are exponentially decreasing in Fourier space.

The main result of [BM14] is the following Theorem.

Theorem 5.3. [BM14] Fix $\sigma \geq 0$ then there exist $R, R' > 0$ s.t. Φ_N is analytic on $B^\sigma\left(\frac{R}{N^\alpha}\right)$ and fulfills

$$\Phi_N\left(B^\sigma\left(\frac{R}{N^\alpha}\right)\right) \subset B^\sigma\left(\frac{R'}{N^\alpha}\right), \quad \forall N \geq 2 \quad (5.5)$$

if and only if $\alpha \geq 2$. The same is true for the inverse map Φ_N^{-1} .

Remark 5.4. A state (X, Y) is in the ball $B^\sigma(R/N^2)$ if and only if there exist interpolating periodic functions (β, α) , namely functions s.t.

$$p_j = \beta\left(\frac{j}{N}\right), \quad q_j - q_{j+1} = \alpha\left(\frac{j}{N}\right), \quad (5.6)$$

which are analytic in a strip of width σ and have an analytic norm of size R/N^2 . Thus we are in the same regime to which Theorem 4.1 apply.

Theorem 5.3 shows that the Birkhoff coordinates are analytic only in a ball of radius of order N^{-2} , which corresponds to initial data with specific energy of order N^{-4} .

We think this is a strong indication of the fact that standard integrable techniques cannot be used beyond such regime.

As a corollary of Theorem 5.3, one immediately gets that in the Toda Lattice the FPU metastable packet of modes is actually stable, namely it persists for infinite times. Precisely one has the following result.

Corollary 5.5. Consider the Toda lattice (5.1). Fix $\sigma > 0$, then there exist constants R_0, C_1 , such that the following holds true. Consider an initial datum fulfilling (4.5) **with** $R < R_0$. Then, along the corresponding solution, one has

$$\mathcal{E}_k(t) \leq R^2(1 + C_1 R)\mu^4 e^{-2\sigma|k|}, \quad \forall 1 \leq |k| \leq N, \quad \forall t \in \mathbb{R}. \quad (5.7)$$

We recall that this was observed numerically by Benettin and Ponno [BP11, BCP13]. One has to remark that according to the numerical computations of [BP11], the packet exists and is stable over infinite times also in a regime of finite specific energy (which would correspond to the case $\alpha = 0$ in Theorem 5.3). The understanding of this behaviour in such a regime is still a completely open problem.

Concerning the FPU chain, Theorem 5.3 yields the following result.

Theorem 5.6. *Consider the FPU system. Fix $\sigma \geq 0$; then there exist constants R'_0 , C_2 , T , such that the following holds true. Consider a real initial datum fulfilling (4.5) **with** $R < R'_0$, then, along the corresponding solution, one has*

$$\mathcal{E}_k(t) \leq 16R^2\mu^4 e^{-2\sigma|k|}, \quad \forall 1 \leq |k| \leq N, \quad |t| \leq \frac{T}{R^2\mu^4} \cdot \frac{1}{|A-1| + C_2R\mu^2}. \quad (5.8)$$

Furthermore, for $1 \leq |k| \leq N$, consider the action $I_k := \frac{x_k^2 + y_k^2}{2}$ of the Toda lattice and let $I_k(t)$ be its evolution according to the FPU flow. Then one has

$$\frac{1}{N} \sum_{|k|=1}^N e^{2\sigma|k|} \omega_k |I_k(t) - I_k(0)| \leq C_3 R^2 \mu^5 \quad \text{for } t \text{ fulfilling (5.8)} \quad (5.9)$$

So this theorem gives a result which covers times one order of magnitude longer than those covered by Theorem 4.1. Furthermore the small parameter controlling the time scale is the distance between the FPU and the Toda

This is particularly relevant in view of the fact that, according to theorem 4.1 the time scale of formation of the packet is μ^{-3} , thus the present theorem shows that the packet persists at least over a time scale one order of magnitude longer than the time needed for its formation.

6 An averaging theorem in the thermodynamic limit

In this section we discuss a different approach to the study of the dynamics of the FPU dynamics, which allows to give some results valid in the thermodynamic limit. Such a method is a development of the one introduced in [Car07] in order to deal with a chain of rotators (see also [DRH13]), and developed in [CM12] in order to study a Klein Gordon chain.

We consider here the case of Dirichlet boundary conditions and endow the phase space by the Gibbs measure at inverse temperature β , namely

$$d\mu(p, q) \stackrel{\text{def}}{=} \frac{e^{-\beta H_{FPU}(p, q)}}{Z(\beta)} dp dq; \quad (6.1)$$

where as usual

$$Z(\beta) := \int e^{-\beta H_{FPU}(p, q)} dp dq$$

is the partition function (the integral is over the whole phase space). Given a function F on the phase space, we define

$$\langle F \rangle \stackrel{\text{def}}{=} \int F d\mu , \quad (6.2)$$

$$\|F\|^2 \stackrel{\text{def}}{=} \int |F|^2 d\mu , \quad (6.3)$$

$$\sigma_F^2 \stackrel{\text{def}}{=} \|F - \langle F \rangle\|^2 , \quad (6.4)$$

which are called respectively the average, the L^2 norm and the variance of F . The correlation of two dynamical variables F, G is defined by

$$C_{F,G} := \langle FG \rangle - \langle F \rangle \langle G \rangle$$

and the time autocorrelation of a dynamical variable by

$$C_F(t) := C_{F, F(t)} , \quad (6.5)$$

where $F(t) := F \circ g^t$ and g^t is the flow of the FPU system.

Remark that the Gibbs measure is asymptotically concentrated on the energy surface of energy N/β , thus studying the system in such a phase space one typically considers data with specific energy equal to β^{-1} .

Let $g \in \mathcal{C}^2([0, 1], \mathbb{R}^+)$ be a twice differentiable function; we are interested in the time evolution of quantities of the form

$$\Phi_g \stackrel{\text{def}}{=} \sum_{k=1}^N g\left(\frac{k}{N+1}\right) E_k .$$

The following theorem was proved in [MBC14]

Theorem 6.1. *Let $g \in \mathcal{C}^2([0, 1]; \mathbb{R}^+)$ be a function fulfilling $g'(0) = 0$. There exist constants $\beta^* > 0$, $N^* > 0$ and $C > 0$ s.t., for any $\beta > \beta^*$ and for any $N > N^*$, any $\delta_1, \delta_2 > 0$ one has*

$$P\left(|\Phi_g(t) - \Phi_g(0)| \geq \delta_1 \sigma_{\Phi_g}\right) \leq \delta_2 , \quad |t| \leq \frac{\delta_1 \sqrt{\delta_2}}{C} \beta \quad (6.6)$$

where, as above, $\Phi_g(t) = \Phi_g \circ g^t$.

This theorem shows that, with large probability, the energy of the packet of modes with profile defined by the function g remains constant over a time scale of order β^{-1} . We also emphasize that the change in the quantity Φ_g is small compared to its variance, which establishes the order of magnitude of the difference between the biggest and the smallest value of Φ_g on the energy surface.

Theorem 6.1 is actually a corollary of a result controlling the evolution of the time autocorrelation function of Φ_g . We point out that, in some sense the time autocorrelation function is a more important object, at least if one is interested in the problem of dynamical foundation of thermodynamics, indeed, by Kubo linear response theory the quantity which enters in the measurements of the specific heat of the chain is exactly the time autocorrelation function.

Remark 6.2. *Of course one can repeat the argument for different choices of the function g . For example one can partition the interval $[0, 1]$ of the variable $k/(N+1)$ in K sub-intervals and define K different functions $g^{(1)}, g^{(2)}, \dots, g^{(K)}$, with disjoint support, each one fulfilling the assumptions of Theorem 6.1, so that one gets that the quantities $\Phi_{g^{(i)}} \stackrel{\text{def}}{=} \sum_k g_k^{(i)} E_k$ are adiabatic invariants, i.e. the energy essentially does not move from one packet to another one.*

The scheme of the proof of Theorem 6.1 is as follows: first, following ideas coming from celestial mechanics, one performs a formal construction of an integral of motion as a power series in the phase space variables. As usual, already at the first step one has to solve the so called homological equation in order to find the third order correction of the quadratic integral of motion. The solution of such an equation involves some small denominators which are usually the source of one of the problems arising when one wants to control the behaviour of the system in the thermodynamical limit. Here we show that, if one takes as the quadratic part of the integral the quantity Φ_g , then every small denominator appears with a numerator which is also small, so that the ratio is bounded. The subsequent step consists in adding rigorous estimates on the variance of the time derivative of the so constructed approximate integral of motion. This allows to conclude the proof.

We emphasize that this procedure completely avoids to impose the time invariance of the domain in which the theory is developed, which is the requirement that usually prevents the applicability of canonical perturbation theory to systems in the thermodynamic limit. Indeed in the probabilistic framework the relevant estimates are global in the phase space.

7 Conclusions

Summarizing the above results, we can say that all the analytic results available nowadays can be split into two groups: the first group consisting of those which describe the formation of the packet observed by FPU and give some estimates on its time of persistence. Such results do not survive in the thermodynamic limit; instead they are all confined to the regime in which the specific energy is order N^{-4} . We find particularly surprising the fact that very different methods lead to the same regime and of course this raises the suspect that there is some reality in this limitation. However one has to say that numerics do not provide any evidence of changes in the dynamics when energy is increased beyond this limit.

A few more comments on this point are the following ones: the limitation appearing in constructing the Birkhoff variables in Toda lattice (which are the source of the limitations in the applicability of Theorem 5.6) are related to the fact that one is implicitly looking for an integral behaviour of the system, namely a behaviour in which the system is essentially decoupled into non interacting oscillators. On the contrary the construction leading to Theorem 4.1 is based

on a resonant perturbative construction in which the small denominators are not present. The main limitation for the applicability of Theorem 4.1 comes from the need of considering the zero dispersion limit of the KdV equation. So, it is surprising that the regime at which the two results apply is equal.

So the question on whether the phenomenon of formation of a metastable packet persists in the thermodynamic limit or not is still completely open. An even more open question is that of the length of the time interval over which it persists. Up to now the best result we know is that of Theorem 5.6, but, from the numerical experiments one would expect longer time scales (furthermore in the thermodynamic limit). How to reach them is by now not known.

At present the only known result valid in the thermodynamic limit is that of Theorem 6.1. However we think that this should be considered only as a preliminary one. Indeed it leaves open many important questions. The first one is the optimality of the time scale of validity: the technique used for its proof does not extended to higher order construction. This is due to the fact that at order four new kind of small denominators appear and up to now we have not been able to control them. Furthermore there is no numerical evidence of the optimality of the time scale controlled by such theorem.

An even more important question is that of the relevance of the result for the foundations of statistical mechanics. Indeed, one expects that the existence of many integrals of motion independent of the energy should have some influence on the measurement of thermodynamic quantities, for example the specific heat. In particular, since the time needed to exchange energy among different packets of modes increases as the temperature decreases one would expect that some new behaviour appears as one lowers the temperature towards the absolute zero. However up to now we have not been able to put into evidence some clear effect of the mathematical phenomenon described by Theorem 6.1. This is one the main goal of our group for the next future.

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